

NASA TECH BRIEF

Lewis Research Center



NASA Tech Briefs announce new technology derived from the U.S. space program. They are issued to encourage commercial application. Tech Briefs are available on a subscription basis from the National Technical Information Service, Springfield, Virginia 22151. Requests for individual copies or questions relating to the Tech Brief program may be directed to the Technology Utilization Office, NASA, Code KT, Washington, D.C. 20546.

Computer Program for Calculation of Complex Chemical Equilibrium Compositions

The problem:

To obtain knowledge of chemical equilibrium composition of a chemical system which would permit calculation of theoretical thermodynamic properties for the system. These properties can be applied to a wide variety of problems in chemistry and chemical engineering.

The solution:

A computer program has been developed to solve numerically, through the use of nonlinear algebraic equations, chemical equilibria in complex systems. A free-energy minimization technique is used.

How it's done:

The program permits calculations such as chemical equilibrium for the following assigned thermodynamic states:

- (1) Temperature and pressure;
- (2) Enthalpy and pressure;
- (3) Entropy and pressure;
- (4) Temperature and volume or density;
- (5) Internal energy and volume or density; and
- (6) Entropy and volume or density.

Other problems capable of being calculated are:

- (1) Theoretical rocket performance;
- (2) Chapman-Jouguet detonations; and
- (3) Shock tube parameter calculations.

The condition for equilibria may be stated in terms of any of several thermodynamic functions such as the minimization of the Gibbs free energy or Helmholtz free energy. If it is desired to use temperature and pressure to characterize a thermodynamic state, the Gibbs free energy is most easily minimized since temperature and pressure are its natural variables. Similarly, the

Helmholtz free energy is most easily minimized if the thermodynamic state is characterized by temperature and volume (or density).

Topics included in the complex equilibrium calculations are: mathematical analysis and techniques for obtaining chemical equilibrium; formulas for obtaining thermodynamic mixture properties and derivatives; criteria for inclusion of condensed phases; calculations at a triple point, inclusion of ionized species; and applications.

Notes:

1. This program is written in FORTRAN IV for IBM-7094 computer and in FORTRAN H for IBM-360. These programs replace previously published computer program LERC-281.
2. Some applications for these programs are the design and analysis of equipment such as compressors, turbines, nozzles, engines, shock tubes, heat exchangers, and chemical processing equipment.
3. Inquiries concerning these programs should be directed to:

COSMIC
112 Barrow Hall
University of Georgia
Athens, Georgia 30601
Reference: LEW-11714 for IBM-7094
LEW-11740 for IBM-360

Source: Sanford Gordon and
Bonnie J. McBride
Lewis Research Center
(LEW-11714) (LEW-11740)

Category 09